

### Abstract

5 The present invention solves the three-dimensional structure of BPI and thereby provides atomic coordinates of BPI from the analysis of x-ray diffraction patterns of sufficiently high resolution for three-dimensional structure determination of the protein, as well as methods for rational drug design, based on using amino acid sequence data and/or x-ray diffraction data provided on

10 computer readable media, as analyzed on a computer system having suitable computer algorithms; and atomic coordinates are provided yielding structural information on related proteins, including the lipid binding and lipid transport protein family that includes BPI, LBP, CETP and PLTP.

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